ZERO TEMPERATURE HOPE CALCULATIONS.

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DISCLAIMER

I. Introduction.

The primary purpose of the HOPE code is to calculate opacities over a wide temperature and density range. It can also produce equation of state (EOS) data. Since the experimental data at the high temperature region are scarce, comparisons of predictions with the ample zero temperature data provide a valuable physics check of the code. In this report we show a selected few examples across the periodic table. Below we give a brief general information about the physics of the HOPE code.

The HOPE code is an 'average atom' (AA) Dirac-Slater self-consistent code. The AA label in the case of finite temperature means that the one-electron levels are populated according to the Fermi statistics, at zero temperature it means that the 'aufbau' principle works, i.e. no a priory electronic configuration is set, although it can be done. As such, it is a one-particle model (any Hartree-Fock model is a one particle model). The code is an 'ion-sphere' model, meaning that the atom under investigation is neutral within the ion-sphere radius. Furthermore, the boundary conditions for the bound states are also set at the ion-sphere radius, which distinguishes the code from the INFERNO, OPAL and STA codes. Once the self-consistent AA state is obtained, the code proceeds to generate many-electron configurations and proceeds to calculate photoabsorption in the 'detailed configuration accounting' (DCA) scheme. However, this last feature is meaningless at zero temperature.

There is one important feature in the HOPE code which should be noted; any self-consistent model is self-consistent in the space of the occupied orbitals. The unoccupied orbitals, where electrons are lifted via photoexcitation, are unphysical. The rigorous way to deal with that problem is to carry out complete self-consistent calculations both in the initial and final states connecting photoexcitations, an enormous computational task. The Amaldi correction is an attempt to address this problem by distorting the outer part of the self-consistent potential in such a way that in the final state after photoexcitation or photoionization the newly occupied orbital sees the hole left in the initial state. This is very important to account for the large number of Rydberg states in the case of low densities. In the next Section we show calculated photoabsorptions compared with experimental data in figures with some rudimentary explanations. 'Experimental data in this case means those of Henke obtainable from the web site www-cxro.lbl.gov/optical_constants/. At the end of the report we provide a list of references.

II. Calculations and Henke Data.

We show a few select cases across the periodic table. The calculations are for isolated atoms (~10^{-5} g/cc) and for solid densities, when those occur. In the HOPE model the distinction between the isolated atom and solid density is important because the boundary conditions for the bound wave functions are given at the ion-sphere radius.

In the HOPE model the main difference between the isolated atom and the same atom at metallic density is twofold; first, the upper level are broadened into bands, which in the case of overlaps changes the level populations, second, if the bands are not filled then the intraband transitions behave like free-free transitions within the band limits and increase the low energy cross sections.

The figures with captions are attached at the end of this report . The Hope data are in black and the Henke in red. The Henke data do not go beyond 30 KeV photon energy. The calculated photoabsorption cross sections together with the Henke data are shown in Figs. 1-7.

In Fig. 8 we show total internal energies and ionization potentials for neutral isolated atoms as computed by the HOPE code and as given by the IPTABLE. IPTABLE is a collection of ionization energies for all elements from Z=1 to 94 in all ionization stages. From IPTABLE total electron energies can be calculated in a straightforward way. In IPTABLE the ionization energies are obtained from James Scofield's self-consistent code [9]. In Fig. 9 we also show the results in green obtained by replacing Scofield's data with the available experimental energies.

Acknowledgement.

References
[1] B. F. Rozsnyai, Phys. Rev. **A5**, 1137 (1972).
[2].A. Goldberg, B. F. Rozsnyai and P. Thompson, Phys. Rev. **A34,** 421 (1986).
[3] B. F. Rozsnyai, S. D. Bloom and D. A. Resler, Phys. Rev. **A44**, 6791 (1991).
[4] B. F. Rozsnyai and M. Lamoureux, JQSRT **43,** 381 (1990).
[5] B. F. Rozsnyai, JQSRT **22,** 337 (1979).
[7] Rozsnyai, B.F. and Einwohner, T. 1982, in *Spectral Line Shapes,* Vol. **2**, 315, **,** ed. K. Burnett
   (Berlin: De Gruyter)
[8] Rozsnyai, B.F. 1977, J. Quant. Spectrosc. Rad. Transf**. 17,** 77.
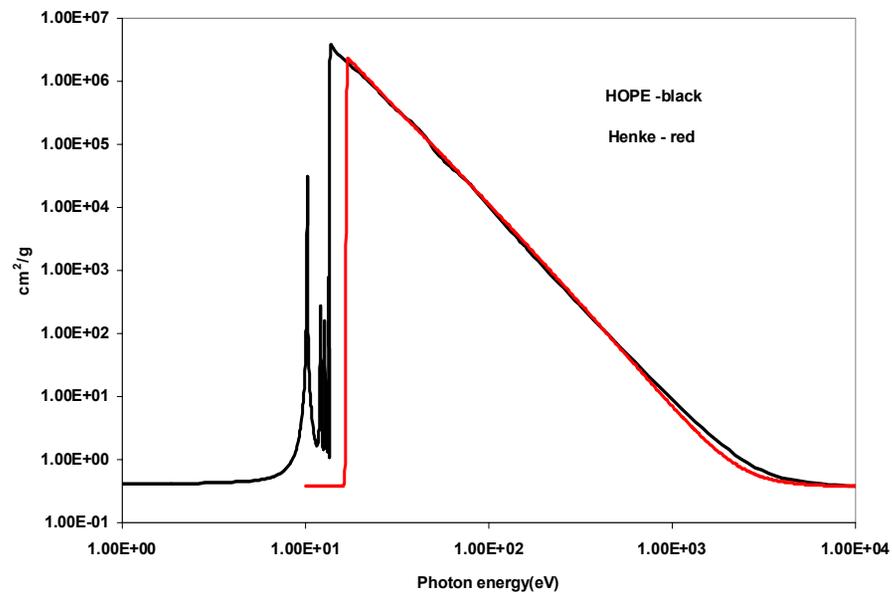[9] James H. Scofield 1973, UCRL-51326, Lawrence Livermore Laboratory report.

Figures.

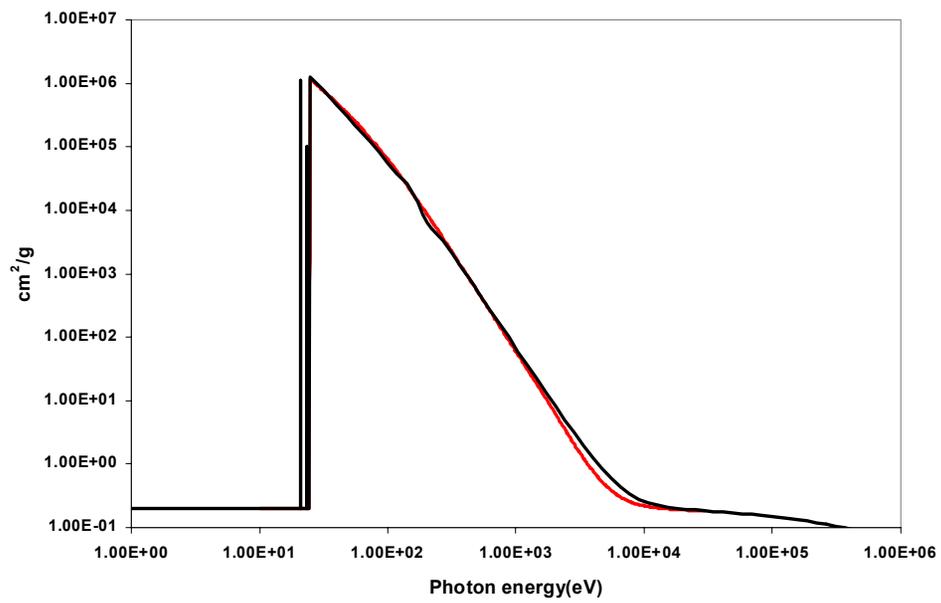Fig. 1. Photoabsorption of hydrogen at kT=0. The Henke data (red) start at 16 eV.
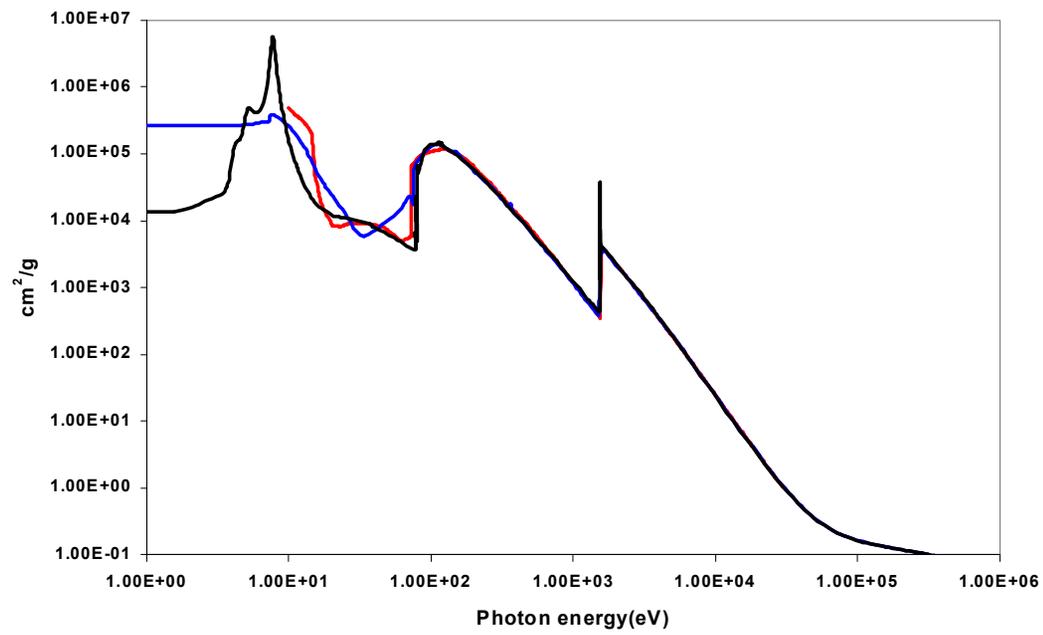
Fig. 2. Same as Fig. 1 for helium.

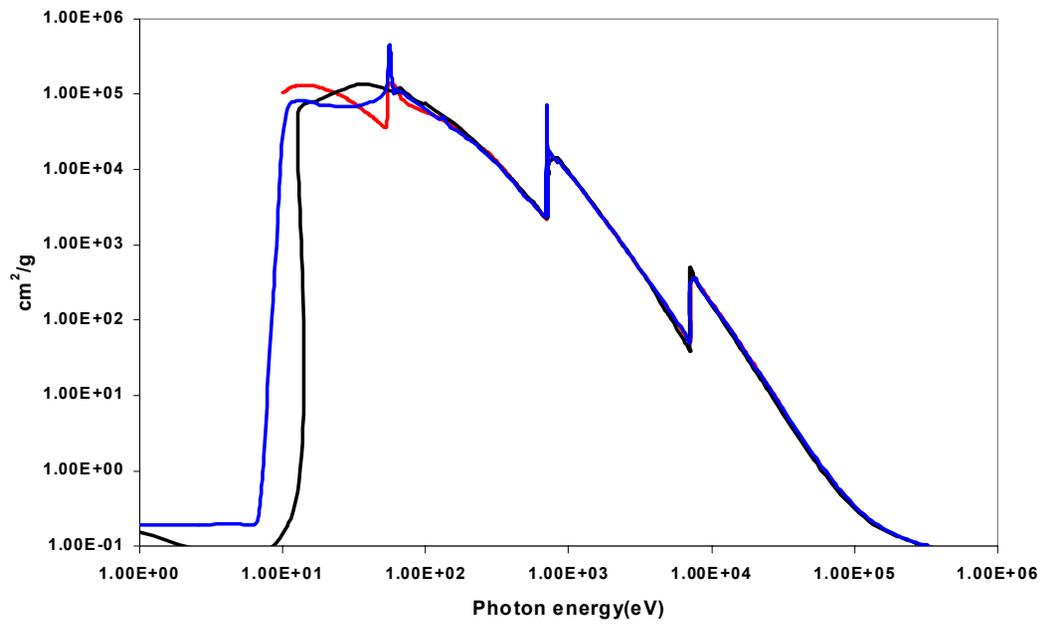Fig. 3. Photoabsorption of isolated (black) and metallic (blue) aluminum at kT=0.

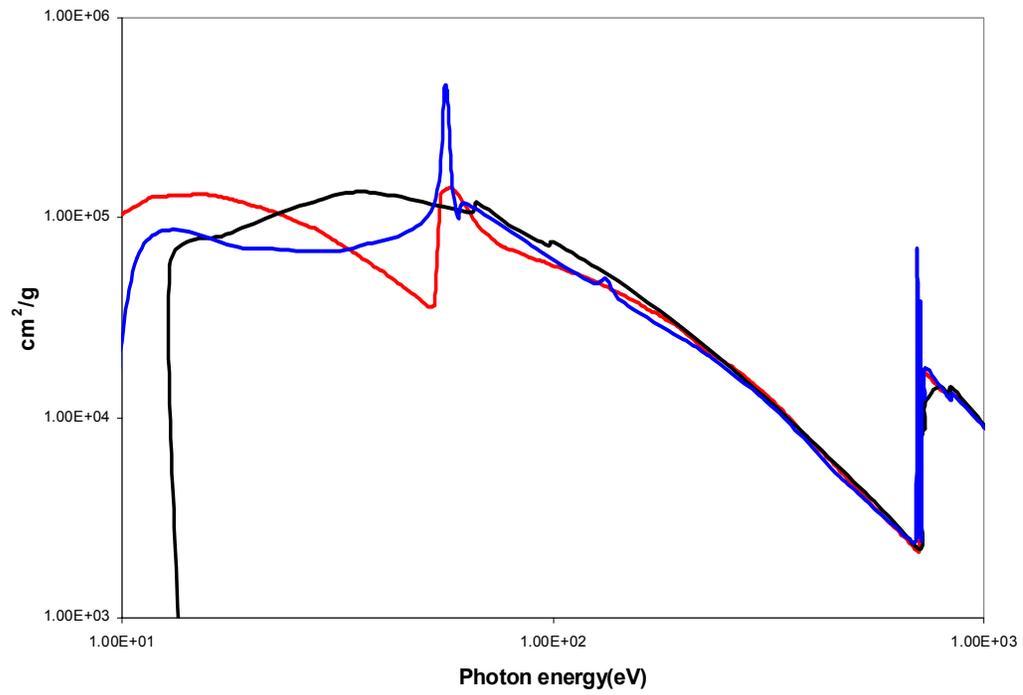Fig. 4a. Photoabsorption of isolated (black) and metallic (blue) iron at kT=0.
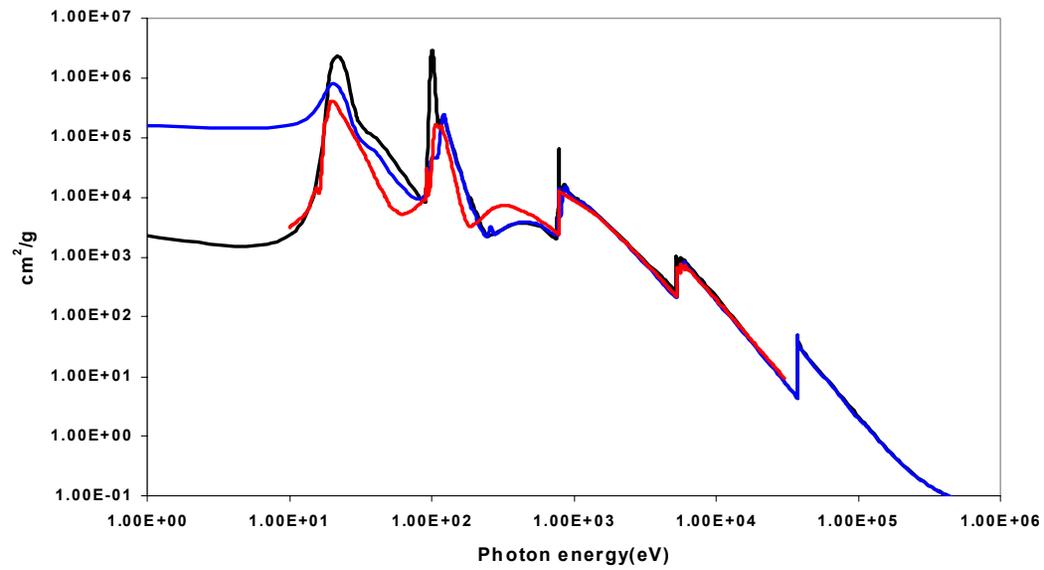
Fig. 4b. Same as Fig. 4a enlarged between 10 eV and 1 KeV.

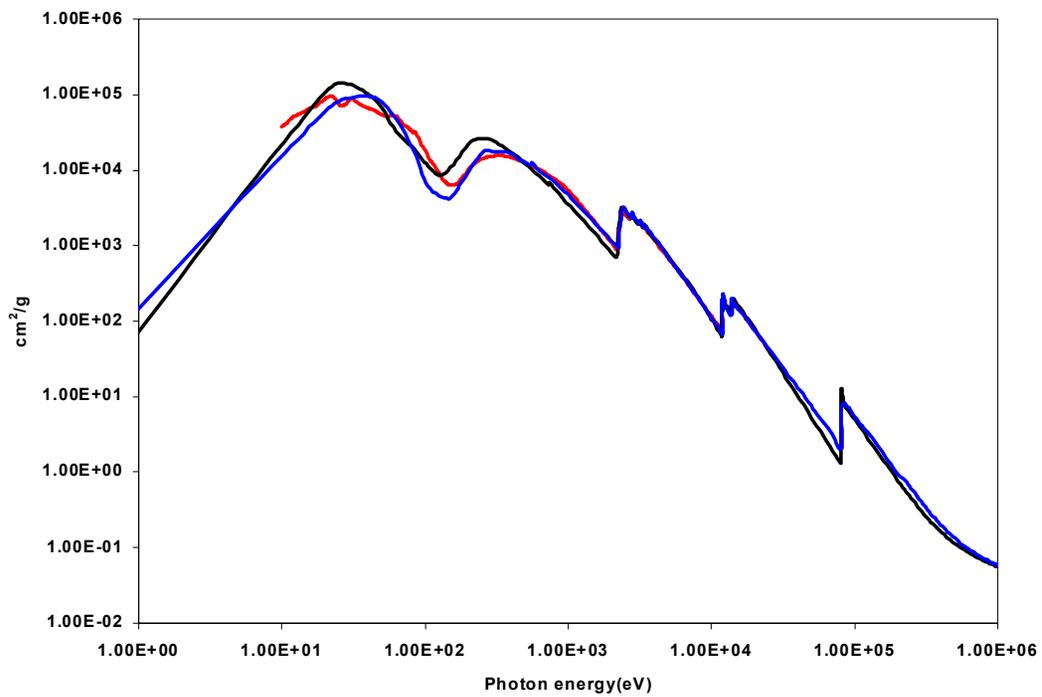Fig. 5. Photoabsorption of isolated(black) and metallic(blue) barium at kT=0.

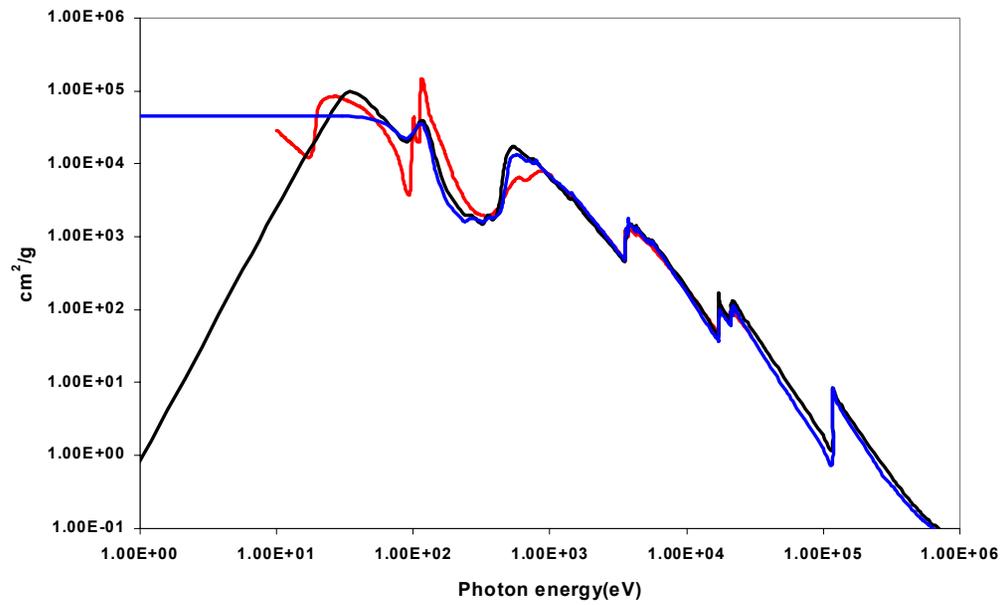Fig. 6. Photoabsorption of isolated(black) and metallic(blue) gold at kT=0

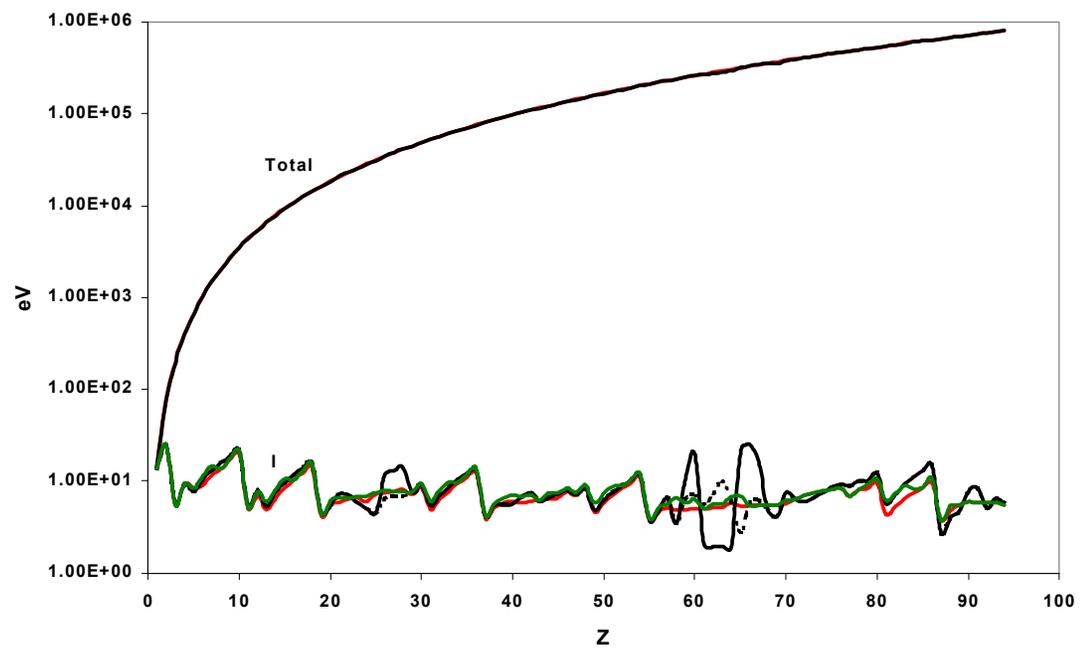Fig. 7. Photoabsorption of isolated(black) and metallic(blue) uranium at kT=0.

Fig. 8. Ionization potential (I) and total electron energies of neutrals given by HOPE (black) and IPTABLE (red). The green curve contains the experimental energies, the red is given by Ref.[9]. The dashed black is a CI mimic by HOPE.